# Noncovalent Interactions within a Synthetic Receptor Can Reinforce Guest Binding

Rodriguez-Docampo, Zaida; Pascu, Sofia I.; Kubik, Stefan; Otto, Sijbren

*Published in:*
Journal of the American Chemical Society

*DOI:*
10.1021/ja062389h



*Publication date:*
2006

**SUPPORTING INFORMATION**

# Noncovalent Interactions within a Synthetic Receptor Can Reinforce Guest Binding

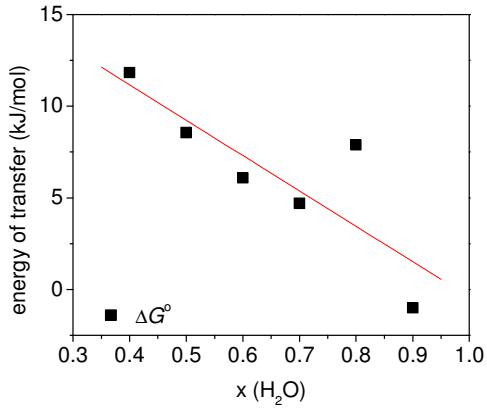
*Zaida Rodriguez-Docampo*[†], *Sofia I. Pascu*[§], *Stefan Kubik**[‡] *and Sijbren Otto**[†]

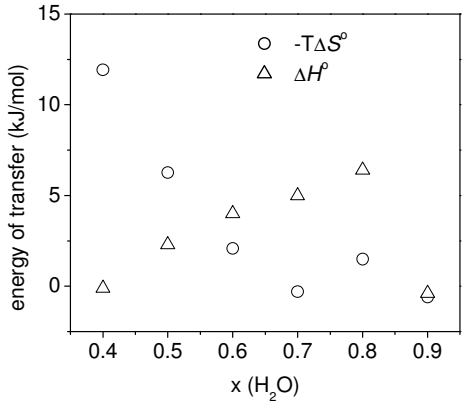
Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge CB2 1EW, United Kingdom, and Fachbereich Chemie - Organische Chemie, Technische Universität Kaiserslautern, Erwin-Schrödinger-Strasse, D-67663 Kaiserslautern, Germany

**Transfer thermodynamics of iodide anion from water to water + acetonitrile**

Data taken from: Hefter, G.; Marcus, Y.; Waghorne, W.E. *Chem. Rev.* **2002**, *102*, 2773-2836.

| | | from Table 42 | at 298.15K | from Table 40 | |
|---|---|---|---|---|---|
| x an (%) | **x $H_2O$** | $\Delta S_t^o$ (J $mol^{-1}$ $K^{-1}$) | **$T\Delta S_t^o$ (kJ $mol^{-1}$)** | **$\Delta H_t^o$ (kJ $mol^{-1}$)** | **$\Delta G_t^o$ (kJ $mol^{-1}$)** |
| 5 | **0.95** | | | **-3.4** | |
| 10 | **0.9** | 2 | **0.596** | **-0.4** | **-0.996** |
| 20 | **0.8** | -5 | **-1.491** | **6.4** | **7.891** |
| 30 | **0.7** | 1 | **0.298** | **5** | **4.702** |
| 40 | **0.6** | -7 | **-2.087** | **4** | **6.087** |
| 50 | **0.5** | -21 | **-6.261** | **2.3** | **8.561** |
| 60 | **0.4** | -40 | **-11.926** | **-0.1** | **11.826** |
| 70 | **0.3** | -43 | **-12.820** | **-3.7** | **9.120** |
| 80 | **0.2** | -40 | **-11.926** | **-8.7** | **3.226** |
| 90 | **0.1** | | | **-11** | |
| 100 | **0** | -88 | **-26.237** | **-9.3** | **16.937** |




Linear fit of data for $\Delta G_t^o$: $\Delta G_t^o = -19 \times$ mol fraction($H_2O$) + 19
So for an increase in the mol fraction of water by 0.1 the $\Delta G_t^o$ from water to a water-acetonitrile mixture becomes less unfavorable by 1.9 kJ/mol. Thus, desolvating iodide becomes 1.9 kJ/mol more costly for every 0.1 increase in the mol fraction of water.